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I. Radiation Transfer and Charge Particle Transport in Gases

Project Coordinator: A. V. Phelps

Radiative Transfer (Dr. D. G. Hummer, Dr. J. Cassinelli, and Mr. P. Kunasz)

Radiation hydrodynamics in spherical geometry. Following the successful solution of the radiative transfer problem in extended spherical systems by Hummer and Rybicki[1*] and the generalization of this method by Cassinelli and Hummer[2] to include effects of non-conservative scattering and polarizations, it became clear that a solution of non-LTE transfer problems coupled with the equations of gas dynamics in a spherical system was feasible and desirable. The basic approach was that of "complete-linearization" -- the iterative solution of a non-linear problem by computing the successive corrections to a linearized version -- as used by Mihalas and Auer in a series of papers[3] to construct non-LTE static models of hot stars. The simplest such problem involves the solution of the equations of mass conservation, momentum and energy, along with the transfer equation for a gray opacity with both scattering and absorption and a steady radial flow. Radiation terms then appear in the energy and momentum equation representing radiation pressure and heating. The transfer equation also acquires terms depending on the flow velocity of the gas.

The major technical point to be faced is the integration of the solution through the critical point, where the flow becomes supersonic. Because of the two-point nature of the boundary value problem for the radiation field, the technique used previously in solar wind calculations of integrating inwards and outwards from the critical point fails in our more general case. When the critical point occurs at large optical depths a "diffusion"

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*References are given at the end of each section.

or "radiative conduction" approximation can be used, as has been done recently by Finzi and Wolf[4] and by Bisnovaty and Kogan.[5] For systems of small optical depth Schmidt-Burgh[6] has developed an inward-outward integration method which becomes unstable for large depths. In the present work the two-point boundary value problem is treated exactly, so that a method of great generality is obtained.

In the first instance the radiation was dropped from the problem in order to develop a stable two-point difference equation procedure for the gas dynamics equation. One of the three boundary conditions is replaced by the requirement that the flow be transonic. A novel scheme for satisfying this requirement at the critical point has been developed. The calculation of the corrections to the linearized equation was found to be stable and efficient. This part of the calculation could be checked by reference to the analytical solution recently published by T. Yeh.

When the radiation is coupled to the gas flow, four equations have to be linearized. At present most of this calculation has been coded and checked, and efforts are concentrated on finding initial trial solutions which are sufficiently accurate to make the computation of corrections possible.

Radiative transfer with migration of excited atoms. As discussed in the previous report, the migration of excited atoms which occurs along with radiative transfer can provide an important energy transfer mechanism. The solution of this problem obtained by Hummer has been coded and checked extensively by Mr. Kunasz. Special attention has been given to the overall energy balance, which holds to better than 1%. It appears that under a wide range of conditions, an important loss of energy occurs through collision of

excited atoms with the walls of the cell.

The important question of when non-radiative transport is significant can be investigated by calculating the mean displacement of an excited atom during its lifetime. If this distance is small compared to the displacement of a typical photon before it is destroyed by a quenching collision of an excited atom, then the non-radiative process can be neglected.

The quenching rate per atom is

$$C_{quench} = \langle vq_{quench} \rangle N_{quench} \equiv t^{-1}_{quench} \quad ,$$

where N_{quench} is the density of the particles responsible for quenching. The rate at which excited atoms suffer elastic collisions with ground state atoms is

$$C_{scatt} = \langle vq_{scatt} \rangle N_1 \equiv t^{-1}_{scatt} \quad .$$

It is well known (cf. Hummer and Rybicki[1]) that a typical photon will experience a displacement (distance perpendicular to the surface) expressed by the so-called thermalization length (on the optical depth scale)

$$\Lambda_r \approx \left(\frac{A_{21} + C_{quench}}{C_{quench}} \right)^n \quad ,$$

where n is 1 for Doppler and 2 for Lorentz broadening.

From random-walk theory, the mean displacement of an excited atom is, on the optical depth scale,

$$\Lambda_a = \lambda_a \langle N \rangle^{\frac{1}{2}} \; k \quad ,$$

where λ_a is the mean free path of the excited atom, $\langle N \rangle$ is the mean number of scatterings experienced by an atom in its lifetime, $k = B_{12}N_1 h\nu_0/4\pi\Delta$ is the absorption coefficient used to calculate the optical depth, Δ is the Doppler or collisional width as appropriate. If we assume that the

mean atomic relative velocity is $\bar{v}$, then for the mean free path we have

$$\lambda_a = \bar{v}\, t_{scatt} \quad .$$

The lifetime of the excited atom is

$$\tau = (A_{21} + C_{quench})^{-1}$$

and the mean number of scatterings is therefore

$$\langle N \rangle = \tau / t_{scatt} \quad .$$

Thus

$$\begin{aligned} \Lambda_a &= \bar{v}\, t_{scatt} \sqrt{\tau / t_{scatt}} \;\; k \\ &= \bar{v}\, k \sqrt{\tau\, t_{scatt}} \\ &= \bar{v}\, k / \sqrt{(A_{21} + C_{quench})\, C_{scatt}} \quad . \end{aligned}$$

If

$$\Lambda_a \ll \Lambda_r$$

the migration of excited atoms can be neglected through the bulk of the gas. However, if excited atoms are quenched by the cell windows, then conditions in regions lying with optical distance of order Λ_a will always differ from those in the purely radiative case. Migration will be particularly important if the primary excitation is concentrated within distance Λ_a of a wall, since the rest of the gas depends on this region for its excitation.

Calculations were carried out for Doppler and monochromatic radiation incident on a plane parallel slab of atoms for which the absorption and emission profiles are characteristic of Doppler broadening. Application has been made to the $^1S_0 \rightarrow {}^3P_1$ transition in Hg (λ=2537 Å) at 400°K. In this case

$\Lambda_r \sim 2 \times 10^3$ and $\Lambda_a \sim 1$, so the calculation showed very little effect of excited atom migration except for $\tau \lesssim 3$. When Λ_a was reduced by artificially increasing C_{scatt}, the region in which migration gave a visible effect was reduced roughly in accordance with the above arguments. Of course, when $\Lambda_a << 1$, then no effect of particle migration could be seen in the emergent radiation.

Atomic Physics (Dr. D. G. Hummer)

A battery of very general atomic physics programs, written by the Atomic Physics Group under Professor M. J. Seaton in the Physics Department of University College London, has been converted to run on the CDC 6400 at the University of Colorado. These programs provide the capability of calculating transition probabilities and electron excitation cross sections for large numbers of transitions in neutral atoms and ions involving orbitals up to 5g, including an arbitrary number of configurations.

The first program does the structure problem and computes transition probabilities by the use of scaled statistical-model potentials. Radial functions are obtained by minimizing the total energy with respect to the scale parameters. This program has been described in detail by Eissner and Nussbaumer.[7] The bound state wave functions from this program can then be used to compute cross sections for electron collisions. For highly charged ions the distorted wave procedure is adequate and allows the rapid calculation of cross sections for all transitions between many terms. For neutral and singly and doubly charged ions, a coupled-equations procedure is more reliable. Professor Seaton completed his coupled-equations code during his stay at JILA this summer, giving us the most efficient such code in existence. Seaton's method is at least an order of magnitude more powerful than

any existing procedure that has been employed so far. We are now in the process of modifying the code to employ fast auxiliary storage, such as Extended Core Storage on CDC computers, to allow very large problems to be solved. It appears that as many as 30 channels can be treated in this way.

Distorted-wave calculations for cross sections in N III, taking into account six configurations with eleven terms, have been completed and work is underway on N IV and N V.

1. D. G. Hummer and G. B. Rybicki, Monthly Notices Roy. Astron. Soc. 150, 419 (1970).

2. J. P. Cassinelli and D. G. Hummer, Monthly Notices Roy. Astron. Soc. (in press).

3. See, for example, D. Mihalas, Stellar Atmospheres (W. H. Freeman and Co., San Francisco, 1970).

4. A. Finzi and R. A. Wolf, Astron. & Astrophys. 11, 418 (1971).

5. Bisnovaty and Kogan, Prikladnaja Matematiki Mehanika, 1967.

6. J. Schmidt-Burgh, Ph.D. thesis, University of Heidelburg, Germany, 1969.

7. W. Eissner and H. Nussbaumer, J. Phys. B 2, 1028 (1969).

Plasma Spectroscopy (Dr. J. Cooper, Dr. J. S. Hildum and Mr. J. Baur)

The final analysis of Ar II and Ca II lines broadened by electrons in the parallel-plate accelerator is now complete.[1,2] Both the Ar II and Ca II results were in good agreement with semi-classical calculations.[3] The Ar II results also agreed well with other experimenters, but (apart from the arc measurements of the French group) the Ca II data were a factor of two larger than previous (mostly shock-tube) measurements. This discrepancy is attributed to the fact that the calcium, which is usually present as an impurity, is not in the hot, dense part of the plasma in the other experiments. These

results, together with detailed numerical experiments, lead us to believe that the semi-classical theory using hyperbolic paths[3] for Stark broadening of ionized species should now be correct to ± 25%,[4] even when the effects of resonance (doubly excited states) are included. A convenient method of analyzing Fabry-Perot profiles when an unknown continuum background is present was developed to obtain the above results.[5]

Development of the C-strap continuum light source has continued, and the effective temperature has been established to be greater than 80,000°K. Used in conjunction with a Z-pinch, the possibility of doing absorption spectroscopy on <u>ionized</u> species is now being actively investigated. In the conventional shock-tube an improved "puffer" now enables an aerosol to be added in a quantitative manner. The Unified theory of line broadening is now being used to generate tables of line profiles of hydrogen broadened by the Stark effect for all important Balmer and Lyman lines. Density and temperatures of interest to the astronomers are being included in this tabulation. A theory has also been developed which will take into account the effect of breakdown of the quasi-static approximation for ions on the forbidden line components in helium[6] and detailed calculations are in progress.

Further work on the broadening due to neutral collisions has shown that the correlation between collisional and Doppler effects is a small effect for most cases of astrophysical interest.[7] However, this formulation[7] also shows how to do calculations in the more interesting "collisional-narrowing" limit, and has clarified the use of action rather than phase integrals in S-matrices for the broadening problems. Line broadening techniques have been applied to the problem of scattering of radiation and a consistent formulation of the frequency redistribution function in the presence of collisions has been obtained.[8]

1. J. S. Hildum, Ph.D. thesis, University of Colorado, 1971.

2. J. S. Hildum and J. Cooper, Phys. Letters (in press).

3. J. Cooper, U. Palmer and G. K. Oertel, JILA Report #105, 1970.

4. R. Bengsten, J. Cooper, and G. K. Oertel (to be published).

5. J. S. Hildum, Appl. Opt. (in press).

6. J. Cooper, E. W. Smith, and W. R. Chappell, Phys. Letters <u>34A</u>, 363 (1971).

7. J. Ward, Ph.D. thesis, University of Colorado, 1971.

8. A. Omont, E. W. Smith and J. Cooper (to be published).

<u>Scattering and Transport of Resonance Radiation</u> (Dr. A. V. Phelps and Dr. J. Jenkins).

The objectives of this project are to experimentally determine a) the magnitude and frequency distribution of radiation scattered by an atom for incident frequencies in the vicinity of a collision broadened resonance line and b) the role of various scattering processes and excitation transfer processes in the transport of the energy of atoms excited to the resonance state. The experimental and theoretical tasks designed to accomplish these objectives include: a) the determination of the frequency dependent absorption coefficients for typical resonance lines as a function of gas, e.g., potassium vapor, density; b) measurement of the spectral intensity of fluorescent radiation in the vicinity of a resonance line; c) the development of theoretical models which correctly describe the spectral distribution of the fluorescent radiation; and d) the development of theoretical models and appropriate experimental tests for the redistribution in frequency which occurs as the result of an individual photon scattering event.

Some measurements of absorption profiles for potassium vapor have been

obtained during this report period. However, no analysis of these data has been undertaken because of the unsatisfactory instrumental profiles for both of the monochromators available for use with this experiment. A computer program has been written and partially tested which will allow a prediction of the contribution of measured instrument profiles to the observed absorption profiles. Since there is little likelihood of obtaining the more ideal instrument profiles shown in the advertising literature in a reasonable length of time, we plan to settle for less than maximum spectral resolution and use the computer program to calculate the distortion of the absorption profiles.

As indicated under the Radiative Transfer project, Dr. Hummer and Mr. Kunasz have obtained accurate solutions for the total intensity and spectral distribution of scattered resonance radiation, i.e., resonance fluorescence, appropriate to low and moderate gas densities where the shape of the spectral line is controlled by Doppler broadening. The results of these calculations have been compared with the experimental measurements by Hansen and Webb[1] of the total intensity of fluorescence of the 2537 Å line of mercury. In agreement with our previous approximate solutions,[2] the inclusion of the destruction of excited atoms at the window explains the data very well. This analysis also shows that the proposed[3] explanation of the data of Hansen and Webb in terms of collisional quenching is incorrect.

The construction of the variable wavelength, pulsed dye laser for use in measurements of the redistribution in frequency resulting when a photon is scattered by an atom has been completed. Tests of the electrical and flow systems are underway and will be followed by test of the optical system and laser operation. As indicated under Plasma Spectroscopy, theories have been developed by Omont, Smith and Cooper, which describe the frequency

redistribution appropriate to the portion of a collision broadened spectral line near line center, i.e., near the limit of our instrumental resolution. It is hoped that these theories can be extended to the wings of the line where experimental testing is easier.

1. J. M. Hansen and H. W. Webb, Phys. Rev. 72, 332 (1947).
2. A. V. Phelps and C. L. Chen, Bull. Am. Phys. Soc. 15, 428 (1970).
3. B. V. Waddell and G. S. Hurst, J. Chem. Phys. 53, 3892 (1970).

<u>Stability of Discharges in Weakly Ionized Gases</u> (Dr. C. J. Hansen, Dr. L. Oster and Dr. A. V. Phelps)

This project was initiated in June 1971 in response to the need for a better understanding of the factors which limit the amount of energy which electrons can transfer to the vibrational and electronic mode of a weakly ionized, molecular gas without producing a transition to a constricted, highly ionized form. We have chosen to investigate the growth of those unstable modes which are thermal in nature, i.e., in which the rise in translation temperature leads to a decrease in molecular density and results in an increase in the electric field to gas density ratio and in the rate of production of electrons. Previous theories[1,2] have considered only steady state solutions or very slowly growing instabilities for which the gas pressure can be considered constant everywhere and are not expected to be applicable to the short duration voltage pulses used in many devices. In addition, some of the solutions[3] predict an unexpected temperature rise near the boundaries of the discharge tube. We have rederived the equations appropriate to the steady state and slowly growing instabilities and are investigating numerical solution techniques. We plan to formulate the

equations appropriate to the initial stages of the faster growing instabilities.

1. G. Ecker, W. Kroll and O. Zoller, Phys. Fluids 7, 2001 (1964).

2. W. J. Wieg, M. C. Fowler and J. A. Benda, Appl. Phys. Letters 16, 237 (1970).

3. A. J. Laderman and S. R. Byron, J. Appl. Phys. 42, 3138 (1971).

Plasma Statistics (Dr. W. E. Brittin and Dr. W. R. Chappell)

Dr. Brittin and Dr. R. H. Stolt have developed a rigorous formulation of the many body problem for composite particles which includes all the proper symmetry related to exchange of particles. In the less rigorous formulation composites are treated as particles having either Bose or Fermi statistics. Thus hydrogen atoms are treated as bosons. However, there is an additional constraint which the states should obey since they should be antisymmetric under the exchange of electrons (or protons) between two atoms. Thus the "physical" Hilbert space is smaller than the "ideal" space in which the atoms are considered simple bosons. The formalism is based on Girardeau's[1] method and gives a fundamental basis for investigating the equilibrium and non-equilibrium properties of systems containing electrons, atoms, ions, molecules, and radiation. A paper describing this method has been published in Physical Review Letters.[2] Dr. Brittin and Dr. Chappell are now making applications of this method to the interaction of radiation and partially ionized plasmas.

A paper by Dr. Chappell and Dr. R. H. Williams of NOAA on the electron diffusion in weakly ionized, magnetized plasmas has been accepted for publication in Physics of Fluids. Experiments to confirm the results have

begun at NOAA. Dr. Chappell and Dr. Williams have been studying the conductivity of weakly ionized gases. A paper describing this work will be submitted for publication in the near future.

1. M. Girardeau, J. Math. Phys. 4, 1096 (1963).

2. R. H. Stolt and W. E. Brittin, Phys. Rev. Letters 27, 616 (1971).

II. Ionization Kinetics and Reaction Rates

Project Coordinator: Dr. W. C. Lineberger

Ionization Kinetics (Dr. W. C. Lineberger, Mr. R. A. Beyer and Mr. T. A. Patterson)

The new flashlamp-pumped dye laser system[1] has been completed and tested. The reliability is much greater than our earlier prototype, and the electrical noise problems are much less severe. Using this laser, wavelength tunability from 5100 Å to 6850 Å has been achieved with the use of only four dyes. The data acquisition system has now been completed, so that we obtain all photodetachment data after each shot of the laser. This system now enables us to sample both the photodetached neutrals and the stripped atom background signal in a time short compared with the coherence time of the ion beam, thereby considerably enhancing the signal-to-noise ratio in the photodetached atom channel.

We have used the sytem to study resonant two-photon photodetachment of electrons from C_2^- ions. This approach represents a unique method for observing intermediate negative ion states. For those states which lie higher than one half of the vertical detachment energy, but below the single photon photodetachment threshold, the apparent photodetachment signal is the product of the bound-bound excitation function and the relatively smooth single photon photodetachment cross section from the intermediate state. The laser power is sufficiently low that only for near resonance pumping of real intermediate states will there be a detectable photodetachment signal.

Figure 1 depicts the C_2^- apparent single photon photodetachment cross section in the wavelength 5300 - 5450 Å, well below the single photon photodetachment threshold, ~3600 Å. The signal-to-noise ratio is ~100 for a

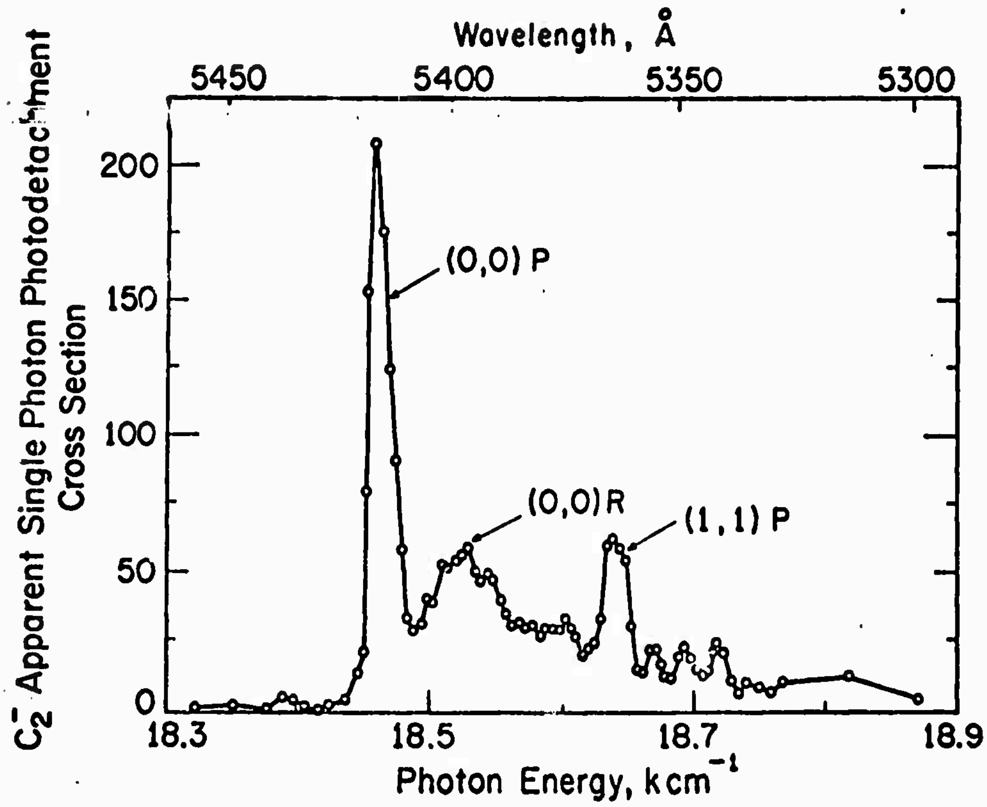

Fig. 1. The C_2^- apparent single photon photodetachment cross section near the $\Delta v = 0$ sequence of the Herzberg-Lagerquist band system. Single photon photodetachment is energetically impossible for photon energies less than ~28,000 cm^{-1}. The indicated P branch peaks appear within ± 2 cm^{-1} of the corresponding P branch band heads of the H-L band system.

100 shot integration at the λ5415 peak. It is immediately clear that these data show a wavelength dependence totally foreign to ordinary bound-free processes. The sharp peaks at λ5415 and λ5363 in fact correspond to P-branch band heads for the (0,0) and (1,1) bands in a $C_2^-\ X^2\Sigma_g^+ \rightarrow D_2^-\ B^2\Sigma_u^+$ transition.[2] These data represent the first positve identification of bound electronic excited states in molecular negative ions, and demonstrate the applicability of resonant two-photon processes to the study of the structure of many molecular ions. Further details may be found in a recent publication.[3]

We have begun to investigate the feasibility of obtaining metal negative ions from our source. We have obtained large (~200 nA) current of Se^- ions from vaporization of SeO_2 in the source discharge, and preliminary photodetachment measurements have been started. The strengths of the line structure transitions observed for Se^- should provide an important test of the photodetachment model presented previously.[4]

Both the Se^- and the two-photon photodetachment studies will be greatly aided by the addition of a Lyot filter[5] to the dye laser, which will reduce the line width to ~.01 cm^{-1}. Construction of the filter is complete, and the system should be operational during the next reporting period.

Superradiance in the dye cell was found to be a significant problem with our nitrogen laser-pumped dye laser used in the molecular fluoresence studies. This problem, however, has been overcome by a modificiation of the dye cell design used by Hansch at Stanford. Our new dye cell, ~2 mm long, permits efficient conversion of N_2 laser light to dye laser light, without the superradiance which usually accompanies high efficiency. We are currently obtaining lifetime data for glyoxal, an intermediate size molecule, as a function both of the exciting wavelength and the fluorescence wavelength.

1. Drawings of the dye laser may be found in D. A. Jennings and D. L. Baldwin, Nat. Bur. Stds. Tech. Note 603, July 1971 (U. S. Government Printing Office, Washington, D. C. 20402).

2. G. Herzberg and A. Lagerquist, Can. J. Phys. 46, 2363 (1968).

3. W. C. Lineberger and T. A. Patterson, Chem. Phys. Letters (to be published).

4. W. C. Lineberger and B. W. Woodward, Phys. Rev. Letters 25, 424 (1970).

5. H. Walther and J. L. Hall, Appl. Phys. Letters 17, 239 (1970).

Molecular Dissociation Processes (Dr. L. J. Kieffer)

A brief summary of our recent results on the dissociative ionization of oxygen, $e + O_2 \rightarrow O^+ + O + 2e$, was presented at the VIIth International Conference on the Physics of Electronic and Atomic Collisions.[1] These experiments are essentially complete and the results will be written up in the near future for publication.

Additional data were taken on the energy distribution and angular distribution of O^- ion from pair formation $e + O_2 \rightarrow O^- + O^+ + e$. The angular distribution observed agreed with the preliminary data taken by R. J. Van Brunt for his thesis. The energy distribution of these ions is a well defined peak centered at about 2 eV ion energy. Study of this process is continuing.

1. L. J. Kieffer, G. M. Lawrence and J. M. Slater, Electronic and Atomic Collisions, (North Holland, Amsterdam, 1971), p. 574.

JILA Information Analysis Center (Dr. L. J. Kieffer)

Compilation and review activities continue in the area of low energy atomic collisions. During this reporting period the following papers were published:

1. "Compilation of Atomic Ultraviolet Photoabsorptive Cross Sections for Wavelengths between 3000 and 10 Å," R. D. Hudson and L. J. Kieffer, Atomic Data 2, 205 (1971).
2. "Low-Energy Electron-Collision Cross-Section Data, Part III: Total Scattering; Differential Elastic Scattering," L. J. Kieffer, Atomic Data 2, 293 (1971).
3. "Critical Review of Ultraviolet Photoabsorption Cross Sections for Molecules of Astrophysical and Aeronomic Interest," R. D. Hudson,

Reviews of Geophysics and Space Physics 9, 305 (1971)..

The following manuscripts were submitted for publication:

1. "Total Electron-Atom Collision Cross Sections at Low Energies - A Critical Review," B. Bederson and L. J. Kieffer (to be published in Reviews of Modern Physics, October 1971).
2. "Ionization and Detachment by Electron Collision," L. J. Kieffer and G. E. Chamberlain (to appear in the DASA Reaction Rate Handbook).

III. Electron Energy Losses and Atomic Interaction Theory

Project Coordinator: Dr. E. C. Beaty

Electron Energy Losses (Dr. E. C. Beaty, Dr. C. B. Opal and Mr. W. K. Peterson)

The ratios of the inelastic scattering cross sections for the n=2 levels of helium to the corresponding elastic scattering cross sections have been measured in a crossed beam apparatus over the 30° to 150° range for incident energies of 82 and 200 eV. At both energies and at angles greater than 40° the ratio of the sum of the inelastic cross sections to the elastic cross section was constant at a few percent, in qualitative agreement with a similar experiment in atomic hydrogen. As shown in Fig. 2, the four n=2 states were observed to have markedly different angular dependencies at 82 eV incident energies. The data of Fig. 3 show that only the ^1S and ^1P states were important at 200 eV; the ratio $^1S/^1P$ was very nearly 2 at all angles larger than 60°. The observed cross sections agreed with those predicted by the first Born approximation to within experimental error only for ^1P at angles less than 45° at 82 eV incident energy and for ^1S and ^1P at 30° and 200 eV incident energy; it appears that other methods must be employed in order to compute cross sections at large scattering angles.

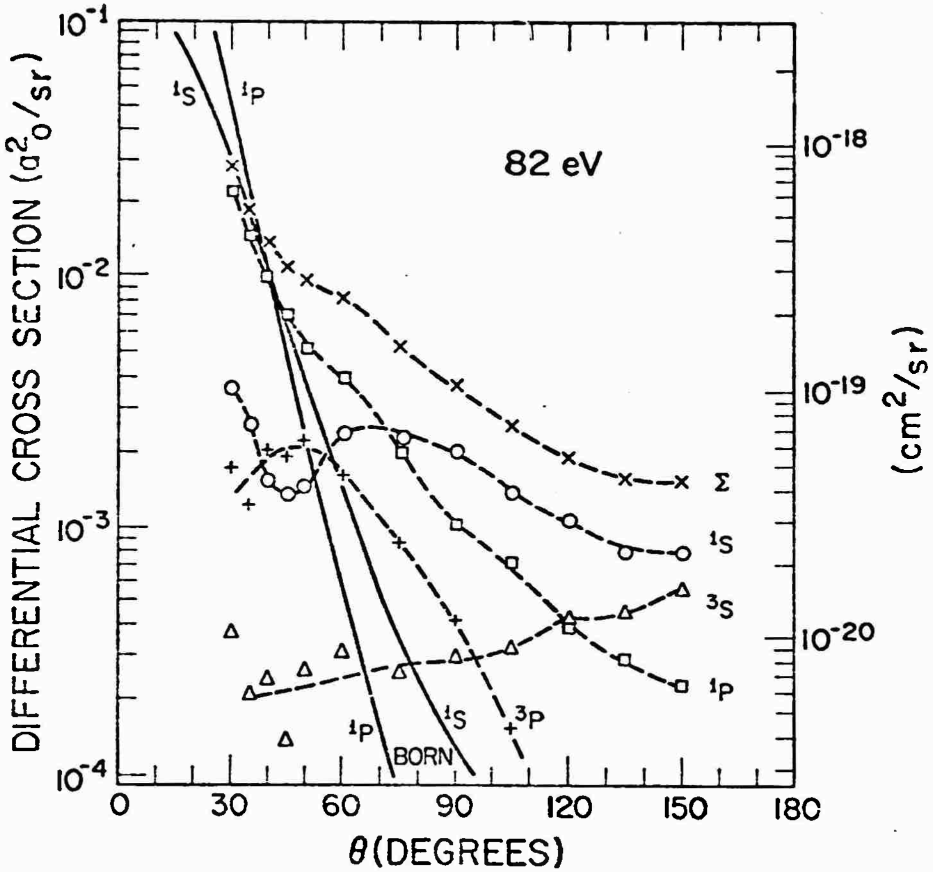

Fig. 2. Experimental results for the excitation of helium expressed in absolute units (---); and predictions of the first Born approximation (——) for 82 eV primaries. Σ refers to the sum of all four inelastic cross sections at the appropriate angle.

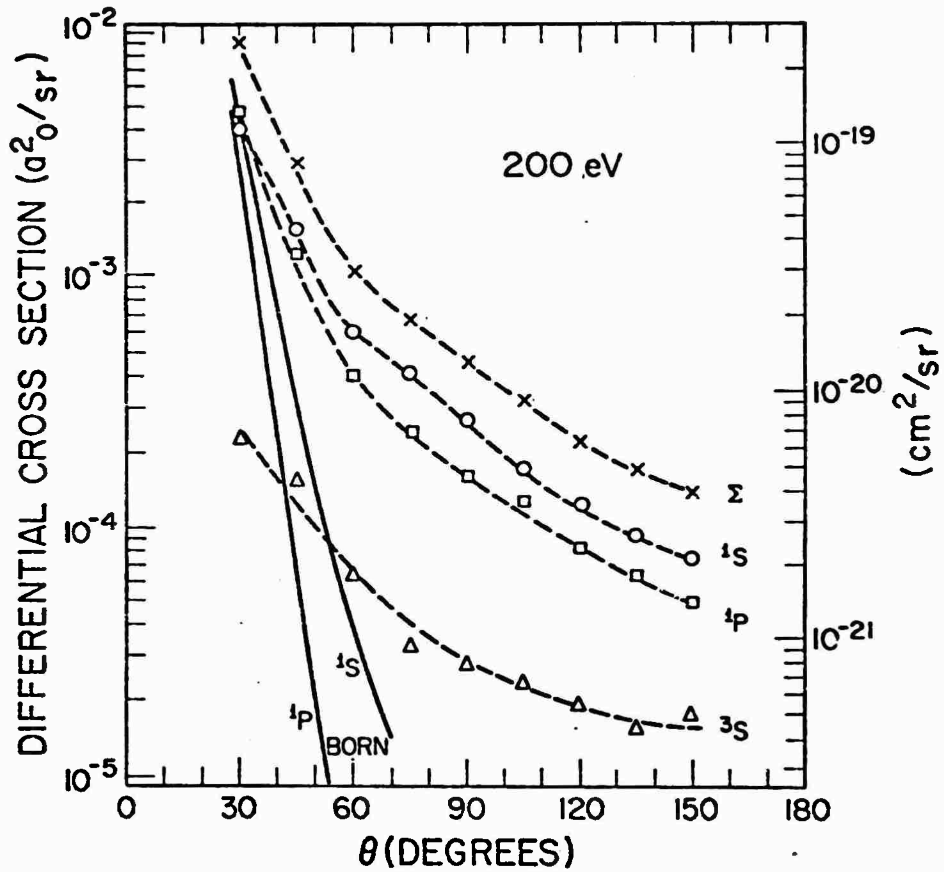

Fig. 3. Experimental results for the excitation of helium expressed in absolute units (---); and predictions of the first Born approximation (——) for 200 eV primaries. Σ refers to the sum of all four inelastic cross sections at the appropriate angle.

Atomic Interaction Theory (Dr. S. Geltman, Dr. D. W. Norcross, and Dr. M. B. Hidalgo)

Fine structure transitions in alkali-rare gas collisions. This project has been completed and a paper on it has been submitted for publication.[1] The results are summarized in Table 1 for the case of Rb in the buffer gases He, Ne, Ar, and Kr. The calculations were done at three relative velocities (v) for each atom pair. The comparison with experiment is made at each v for the inelastic ($j=1/2 \to 3/2$) cross sections, and with a thermally averaged ($\bar{v}$) experimental value for the depolarization ($j=1/2; m=1/2 \to -1/2$) cross sections. The one adjustable parameter in the theoretical mode is R_0, a hard sphere radius which determines the assumed trajectories. The optimum values of R_0 are those which result in the best overall agreement between the calculated and measured[2] values for σ_I and σ_D.

Table 1

Rare Gas	$v(10^5 cm/sec)$	Optimum $R_o(a_o)$	$\frac{v}{\bar{v}}$	$\frac{\sigma_D \text{ Theory}(v)}{\text{Exp}(\bar{v})}$	$\frac{v}{v_{th}}$	$\frac{\sigma_I \text{ Theory}(v)}{\text{Exp}(v)}$
He	2.5	7.2	1.8	.65	2.1	5.6
He	3.0	7.1	2.1	.65	2.5	5.1
He	4.0	6.6	2.8	1.0	3.3	2.9
Ne	2.0	10.0	2.9	.80	3.4	7.1
Ne	3.0	9.7	4.4	1.1	5.1	5.9
Ne	4.0	9.3	5.9	1.5	6.8	3.4
Ar	1.5	12.2	2.8	.34	3.3	9.0
Ar	2.0	12.1	3.8	.47	4.4	4.9
Ar	2.5	11.9	4.7	.60	5.5	2.8
Kr	1.5	13.7	3.6	.31	4.1	2.7
Kr	2.0	13.5	4.8	.42	5.4	1.1
Kr	2.5	13.3(5)	5.9	.55	6.8	1.0

The depolarization cross sections agree with experiment to within a factor of 3 at all velocities calculated, while the inelastic cross sections agree with experiment to within a factor of 9. This is for a set of measured

cross sections which have a spread in magnitude of about a factor of 300. All of the σ_T and most of the σ_D theoretical values improve as the energy is increased, such that at the highest energies calculated we obtain agreement with all measured cross sections to within a factor of 3. The otpimum values of R_0 are appreciably larger than the repulsive radii of the adiabatic potential curves calculated by Baylis.[3]

A Coulomb-projected Born approximation for high energy collisions. The work on this approximation applied to proton-hydrogen charge transfer and hydrogen atom excitation by electrons has been completed and two papers on it have been accepted for publication.[4] The conclusion that the Born approximation is grossly inadequate for predicting high energy electron-atom inelastic differential cross sections has been further experimentally substantiated by work of Opal and Beaty on the excitation of helium (see Electron Energy Loss section).

We are currently applying our present approximation to the 2^1S and 2^1P excitation of helium by electrons. The wave functions being used are:

$$\Psi(1^1S) = \Psi_{1s}(r_1)\Psi_{1s}(r_2); \quad \Psi_{1s} = N(e^{-\alpha r} + \eta e^{-\beta r})$$

$$\Psi(2^1S) = N\left[\phi_{1s}(r_1)\Psi_{2s}(r_2) + \phi_{1s}(r_2)\Psi_{2s}(r_1)\right] ;$$

$$\phi_{1s} = \text{ground state hydrogenic } (Z=1)$$

$$\Psi_{2s} = N(e^{-\alpha' r} + \eta r e^{-\beta' r})$$

$$\Psi(2^1P) = N\left[\phi_{1s}(r_1)\phi_{2p}(\vec{r}_2) + \phi_{1s}(r_2)\phi_{2p}(\vec{r}_1)\right] ;$$

$$\phi_{2p} = 2p \text{ hydrogenic } (Z=0.97) .$$

The adequacy of these atomic functions has been tested by calculation of the Born cross sections for them and comparing with Born results using much more elaborate, correlated wave functions.[5] The very close agreement between these two Born results tells us that the simple analytic wave functions above are quite good for this purpose.

Lyman-α line shape. the object of this study is to evaluate the line shape one would expect from the binary interaction of hydrogen atoms with electrons. The absorption coefficient for continuous radiation of frequency ν near the Ly-α frequency (ν_0) is proportional to

$$\left|\iiint d\vec{r}_1 d\vec{r}_2 \; \Psi^*_{1s\vec{k}}(\vec{r}_1,\vec{r}_2) \; (\vec{r}_1+\vec{r}_2) \; \Psi_{2p\vec{k}'}(\vec{r}_1,\vec{r}_2)\right|^2$$

where $h(\nu-\nu_0) = k'^2 - k^2$, and $\Psi_{1s\vec{k}}$ and $\Psi_{2p\vec{k}'}$ are the electron-atom scattering wave functions in which the incident electron has wave vectors $\vec{k}$ and $\vec{k}'$, and the atoms are in the 1s and 2p states, respectively.

Much past effort has gone into the development of improved electron-hydrogen wave functions by the means of close coupling and pseudo-state expansions. A significant amount of this was done here under the present ARPA contract.[6] The use of these wave functions in the above dipole intergral should provide the most accurate values presently available for that integral.

During this report period we have completed the computer codes to do all the angular and radial integrals required. The close coupling codes to obtain the scattering wave functions are being rewritten in a form developed by Prof. M. J. Seaton which will cut down the required computer time by an order of magnitude. The computer time required will still be very large, and a request for free computer time on the NCAR CDC 7600 has been made.

Elastic scattering and photoionization. Work has been completed on a calculation of the photoionization cross section of the metastable states of He. Solutions of the multi-channel coupled equations for e-He^+ scattering were used as final states. Oscillator strengths for photoexcitation of the lowest few resonance states of He were also obtained. This work has been published.[7]

Work is in progress on a calculation of the photoionization cross sections of the ground and metastable states of Mg using similar techniques. Extension to Ca and Ba is contemplated.

A study was performed of very low energy elastic scattering of electrons by Li and Na, and it was found that resonance structure previously reported was the consequence of numerical instability in previous numerical work. The low energy spin-exchange cross section for e-Na collisions was found to differ substantially from experimental determinations. A report on this work has been accepted for publication in J. Phys. B. Accurate calculations of elastic and inelastic processes at higher energies in e-Na scattering have also been completed. A report on this work with Dr. D. L. Moores will shortly be submitted for publication. Extension of this work to the heavier alkalis and alkaline earths, particularly Cs and Ba^+ is in progress.

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2. A. Gallagher, Phys, Rev. 157, 68 (1967); Phys. Rev. 172, 88 (1968).

3. W. E. Baylis, J. Chem. Phys. 51, 2665 (1969).

4. S. Geltman, "A high energy approximation I. Proton-hydrogen charge transfer"; S. Geltman and M. B. Hidalgo, "A high energy approximation II. Hydrogen atom excitation by electrons," J. Phys. B: Atom. Mol. Phys. (in press).

5. K. C. Bell, D. J. Kennedy, and A. E. Kingston, J. Phys. B 2, 26 (1969); Y. K. Kim and M. Inokuti, Phys. Rev. 175, 176 (1968).

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IV. Electron-Atom Collisions

Project Coordinator: Dr. S. J. Smith

Excitation of Ions by Electron Impact (Dr. G. H. Dunn, Dr. K. Dolder, Dr. W. E. Kauppila, and Mr. P. O. Taylor)

This project is to measure the cross sections for electron-impact excitation of N_2^+, Ca^+, and Ba^+ using crossed beams of variable energy electrons and the respective ions and observing the resultant resonance radiation along the third perpendicular direction. Preliminary results were reported earlier.

The period covered by this report was spent in refinements of the experiment preparatory to obtaining final, accurate absolute values of the respective cross sections. The effort is highlighted by two main accomplishments:

1) Absolute radiometric calibration of the apparatus. For this a uniform, isotropic source of monochromatic light was constructed, and its radiance measured by careful comparison with a copper point black body. The calibrated source was then used to calibrate the absolute sensitivity of the crossed beam apparatus for each of the 5 wavelengths of the various ions. The spatial variation of the sensitivity of the apparatus was also measured using a similar source, so that when used with the above absolute calibration and folded with the respective beam spatial distributions, an absolute cross section can be extracted.

2) Electron gun modification and evaluation. The electron gun used for this experiment is of a magnetically confined variety. This is necessitated by the fact that target densities for the collisions under study are only of the order $10^5/cm^3$ and light detection sensitivity is only about

10^{-3}. It is thus necessary to have a magnetically confined gun to insure adequate current at threshold electron energies (2 to 3 eV) for the processes under study. Such a gun, however, is subject to severe criticism based on the fact that the electron trajectories are cycloidal in nature, and determination of the actual electron path length through the target is uncertain. However, a technique to measure the amount of spiraling -- and hence path length increase -- was developed during the report period, and the gun was tested and modified so that corrections for path length ranging up to only 3% are necessary. This is contrasted to corrections and uncertainties of several tens of percent if improper gun conditions are used. Though much careful effort has previously gone into evaluating such guns, this is believed to be the first direct test and measurement of the effect.

Final absolute measurements of the respective cross sections are now being made along with calibration "rechecks."

Electron Collisions with Metastable Atoms (Dr. G. H. Dunn and Dr. W. E. Kauppila)

This program is to measure electron impact excitation and ionization of H(2S). Major relevant apparatus additions had been built and tested prior to beginning of this report period. Since further progress on this experiment involves use of the apparatus being used for electron-ion excitation, no further work was done on this experiment during the report period.

Electron-Ion Recombination (Dr. F. L. Walls and Dr. G. H. Dunn)

A new technique is being developed for the study of electron-ion collisions. First studies are of the dissociative recombination of elec-

trons and molecular ions contained in an axially symmetric quadrupole ion trap of the Penning variety.[1] The stored ion gas will be irradiated with a beam of electrons and the number of remaining ions vs time nondestructfully measured. The absolute number of ions, their spatial distribution, the electron beam intensity, and its spatial distribution will be measured using a Bendix Spiraltron Bundle Detector. These measurements are sufficient to determine the cross section for a given electron energy and distribution or ion vibrational levels. The electron energy range will extend from about 30 meV to several (4 or 5) eV. The first ions to be studied will be NO^+ and N_2^+.

This approach allows one to separately investigate the effects of the interaction energy (which is previously determined by the electron energy) and the distribution of occupied vibrational levels, on the cross section. The long storage times and high e/m resolution of the trap and detection system eliminate uncertainties due to excited electronic states which occur in the ion creation process, and the contamination of the sample with unwanted ions.

The trap and all the electronics necessary to store and detect ions have been built, and preliminary tests of the trap and associated electronics are under way. Trapped electrons rather than ions are used in the preliminary test and alignment because the detection sensitivity is higher for electrons. The homogeneity of the magnetic field in the trap has been measured to be better than 1 ppm, a requirement for long ion lifetimes. Tests have shown that holes in the trap electrodes which allow the electron beam to pass through the trap also permit electric fields from the electron gun to penetrate the trap, thus causing unacceptable perturbations to their axial motion. (In order to permit easier modifications of the trap and the

electron gun a special nonmagnetic demountable stem was constructed.) The holes in the trap electrodes have been shielded and/or covered with fine wire screen, and further testing of the storage capabilities of the trap will now be resumed.

Modifications have also been made to the electron gun assembly. The gun now delivers 1×10^{-10} amps with 30 meV FWHM. This is a substantial improvement over the original design.

A detailed investigation of vibrational relaxation times indicates that for the ion density obtainable in the trap the vibrational relaxation times for homonuclear ions (even in the presence of electric fields) are much longer than the expected trapping lifetime of the ions. However, for ions like $N_{14}\,N_{15}^+$, HD^+ NO^+ etc. the relaxation times are typically less than a few seconds. The vibrational temperature is determined by the temperature of the radiation off the walls the trap. Although not as easily manipulated as the noise temperature of the tank circuit it is possible to change the vibrational temperature in a carefully calibrated manner.

Based on data using electrons, the trap characteristics are such that one can easily distinguish between molecular ions with masses one mass unit apart in the mass range for NO^+, N_2^+, etc. One can destroy every other value of charge to mass ratio except the one desired for study.

With completion of modifications to the trap electrodes mentioned above, we will begin testing the heavy ion trapping characteristics of the trap. With success here, we can obtain relative cross section measurements over the electron energy range mentioned. Development of the channeltron bundle detector system mentioned above will continue, and with this, absolute cross sections will be forthcoming.

1. H. G. Dehmelt, Advances in Atomic and Molecular Physics (Academic Press, Inc., New York, 1967), Vol. 3, p. 53.

Electron-Alkali Atom Scattering (Dr. S. J. Smith, Dr. M. V. McCusker and Mr. D. Hils)

This experiment involves the elastic scattering of low energy electrons from polarized potassium. Disregarding spin-orbit effects and hyperfine interactions during the collision the differential scattering cross section, in terms of the direct $[f(\theta, \phi)]$, and exchange $[g(\theta, \phi)]$ amplitudes, is written

$$\sigma(\theta, \phi) = 1/2|f(\theta, \phi)|^2 + 1/2|g(\theta, \phi)|^2 + 1/2|f(\theta, \phi) - g(\theta, \phi)|^2 \quad .$$

The quantity $|f|^2/\sigma$ can be determined[1] by scattering unpolarized electrons from an initially polarized alkali beam and measuring the polarization of the scattered electrons over a range of scattering angles. Thus if P_e is the measured electron polarization, and P_A is the initial atomic polarizations, the measurement yields

$$|f(\theta, \phi)|^2/\sigma = (1 - P_e/P_A) \quad .$$

During the period covered by this report we obtained data for several angles at one energy (4 eV). This experimental program complements other investigations, by Bederson and co-workers,[2] which determine the ratio $|g|^2/\sigma$. We also made measurements of relative angular distributions which, when properly normalized yield the differential scattering cross section $\sigma(\theta, \phi)$; these were reported at a recent APS meeting.[3] Our measurements can be compared with theoretical computations which utilize the close coupling approximation.[4,5]

The experimental apparatus was described in the previous report and the discussion will not be repeated.

The results of our measurements of electron polarization at 4 eV electron energy are shown in Table 2. The errors in this measurement are primarily statistical in nature; a typical counting rate (at 40°) for this double scattering measurement is 2 counts/sec while the background counting rate is about 10 counts/sec. Also shown in the table are values of $|f|^2/\sigma$ computed from these data; these are then plotted in Figure 4. The continuous curve in that figure was computed from the K matrices published by Karule.[5] It appears that our points fall off more rapidly with increasing angle than does the theory. We shall continue our measurements at larger angles but these are difficult since the scattering cross section is very small.

Table 2

Scattering Angle θ

	20°	30°	35°	40°
P_e	-0.013 ± 0.023	+0.060 ± 0.048	+0.036 ± 0.036	+0.193 ± 0.073
$\|f\|^2/\sigma$	1.06 ± 0.12	0.70 ± 0.23	0.82 ± 0.18	0.03 ± 0.33

During the next reporting period we shall make extensive modifications to most of the apparatus used in the elastic scattering experiment; the goal of these modifications will be automation of the data taking process to permit a significant reduction in statistical uncertainties.

While these alterations are being made we shall study the circular polarization of resonance radiation arising from electron impact excitation of polarized potassium. This will allow us to investigate spin exchange

processes in inelastic collisions. The spectrometer and polarization analysis system for these studies have already been installed on the apparatus.

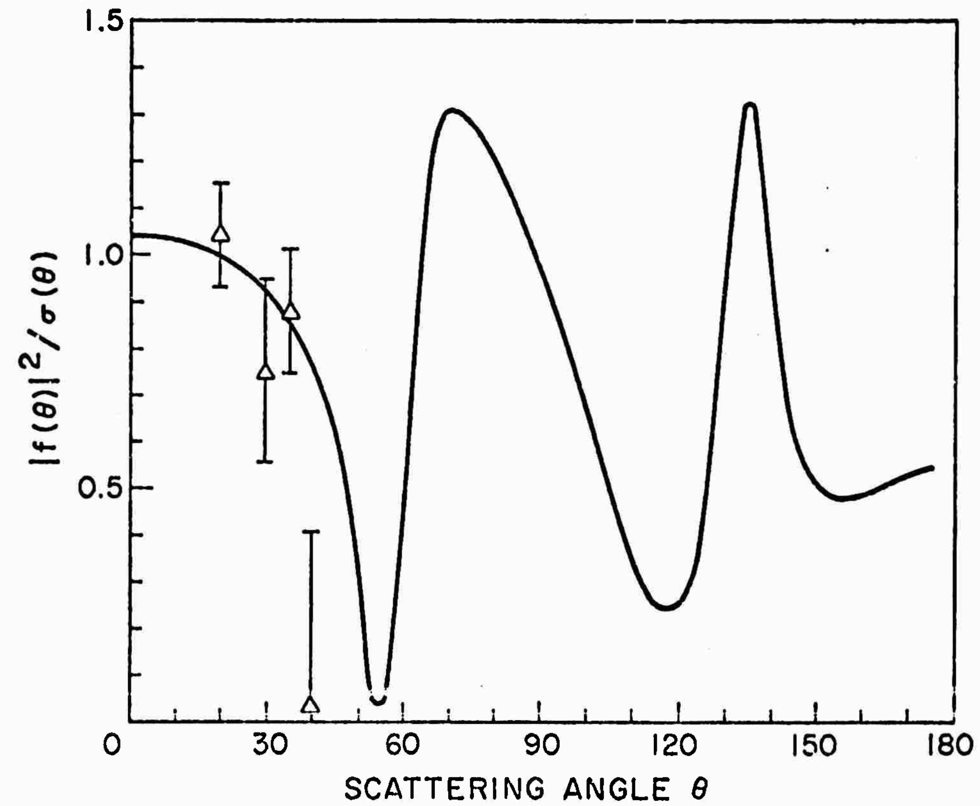

Figure 4

1. Complete discussions of the many possible spin-dependent experiments that can be done with electron-alkali atom collisions can be found in B. Bederson, Comments Atomic Mol. Phys. 1, 41 (1969); H. A. Kleinpoppen, Phys. Rev. A (in press).

2. R. E. Collins, B. Bederson, M. Goldstein and K. Rubin, Sixth ICPEAC: Abstracts of Papers (MIT Press, Cambridge, Mass., 1969) p. 781; also Phys. Letters 27A, 440 (1968).

3. D. Hils, M. V. McCusker, H. A. Kleinpoppen and S. J. Smith, Bull. Am. Phys. Soc., 16, 587 (1971).

4. P. Burke and J. Taylor, J. Phys. B. 2, 869 (1969).

5. E. M. Karule and R. K. Peterkop, in Atomic Collisions III, (Y. Ia. Veldre, Ed., Latvian Academy of Sciences, Riga, USSR, 1965). [Translation: JILA Information Center Report #3, University of Colorado, Boulder, Colorado (unpublished) p. 1-28].

Collisional Relaxation Mechanisms (Dr. P. L. Bender and Mr. R. Brill)

The history of work on this project was reviewed at length in the last semi-annual report. Work was suspended at the end of January, 1971 until completion of calculations on the expected signal in transmitted light for the high-field experiment. It has since been found that new theoretical work would be needed in order to permit completion of the calculations. In view of budget limitations and the present lack of evidence that Xe would be better than Hg for use in a nuclear gyroscope, a decision to terminate this project was made. No funds were spent on the project during the present reporting period.

V. Radiation Processes

Project Coordinator: Dr. A. C. Gallagher

Collisional Radiation (Dr. A. C. Gallagher)

The theory and data on the Cs far wing emission spectra, due to interaction with inert gases, have been prepared for publication. This yields detailed information on the interaction potentials for the ground ($X\ ^2\Sigma$) and excited ($A\ ^2\Sigma_{1/2,3/2}$ and $B\ ^2\Sigma$) molecular states and on the continuum absorption and emission between 8000 and 10,000Å for the Cs-inert gas system.

The high-luminosity scanning Fabry-Perot interferometer has been improved in through-put and reliability, and the system has been prepared for measurements on the extreme wings of the Rb resonance lines. A considerable increase in sens'tivity has been achieved over the previous measurements and it should now be possible to measure the three-body molecular formation rates (of Rb-inert gas molecules) and vibrational transitions for the $A\ ^2\Pi_{1/2 \text{ and } 3/2}$ states. The adiabatic potentials should also be established by the measurements, as in the Cs case.

Polarized Radiation (Dr. A. C. Gallagher)

Preliminary work has been done on a review of laboratory studies involving polarized fluorescence. Radiative diffusion and collisional destruction of the polarization are discussed. Theories for resonance and polarization signals, which relate the laboratory observables to the collision and diffusion processes, are also covered.

Negative Ion Studies (Dr. J. Hall, Dr. R. Celotta, Mr. R. A. Bennett)

The analysis of the O_2^- and NO^- photodetachment data is now complete.

A proper deconvolution of the experimental data to recover the fundamental molecular parameters turned out to be much more complicated than originally expected. The basic problem area is the treatment of rotational temperature:

1) How does one handle the finite cutoff region where the rotational energy of the negative ion is about equal to the electronic potential well depth? (Luckily our source temperature of 630°K is low enough that only about ±2 millivolts uncertainty in the affinity results from the two limiting assumptions.)

2) What are the precise angular momentum selection rules for photodetachment? From first principles, the total angular momentum may change only by 0, ±1 units of $\hbar$. However, the rotational energy is associated only with a certain component of the total angular momentum. Detailed consideration leads to the conclusion that Hund's case (a) is appropriate, and that our problem is probably bounded by the intensity ratios between P-, Q-, and R-branch transitions of 1:2:1 to 1:10:1. We have completed numerical convolution of the spectrometer function with the theoretical spectra under these two limiting intensity assumptions with consideration of the rotational distribution function mentioned before. Fine structure splitting of both negative ion and final neutral molecule states is taken into account. The resulting "theoretical" line shape is then characterized by the slightly-skewed Gaussian fitting function which is used to characterize the data.

Both the NO^- and O_2^- results have now been prepared for publication.

A new argon laser has been put into operation. The resulting increase in power and reliability will allow us carefully to measure a variety of interesting negative ions. The 3511Å transition available with this laser, along with our increasing sophistication in the analysis of molecular photo-

detachment data should allow meaningful investigation of the simpler strongly bound negative ions of atmospheric interest.

Preliminary measurements have been made on the NH^- and NH_2^- molecules as well as S_2^-, SO^- and SO_2^-. Now that the ion source techniques are increasingly under control for these species we can carry out the systematic measurements and analysis necessary to obtain the affinities and vibrational structure of these molecules.

Oscillator Strengths and Transition Probabilities (Dr. R. H. Garstang)

Calculations have been continued on transition probabilities of allowed and forbidden lines for a number of atoms and ions of particular interest. One set of calculations concerned forbidden transitions within the ground configurations of the atom of the C I isoelectronic sequence. These had first been calculated nearly forty years ago, and refined calculations had been published[1] in 1951. None of these early results included the effects of configuration interaction explicitly, though it had been hoped, and partially justified,[2] that the methods employed using empirical values of the energies of the atomic levels would take into account at least part of the unknown effects of configuration interaction. Computing facilities make it possible to study the effect of configuration interaction in much more detail, and the calculations on the C I sequence were repeated, including four configurations, $2s^2 2p^2$, $2p^4$, $2s^2 3d^2$ and $2s2p^2 3d$. The new transition probabilities[3] do not differ from the earlier ones by more than 30%. This enhances our trust in the reliability of other transition probability data for forbidden lines, confirming our conclusion from earlier work on Fe I and Fe II forbidden lines. However, some of the differences, even if less than 30%, may perhaps have some significance, especially where ratios of

lines are under consideration and experimental values of the ratios may be determinable to a greater accuracy than 30%.

1. R. H. Garstang, Monthly Notices Roy. Astron. Soc. 111, 115 (1951).
2. R. H. Garstang, Proc. Camb. Phil. Soc. 52, 107 (1956).
3. H. Nussbaumer, Astrophys. J. 166, 411 (1971).

Manuscripts Involving ARPA Funds

Listed below are papers submitted for publication during the period covered by this report. Co-authors not connected with JILA are shown in parentheses.

E. C. Beaty, C. B. Opal and W. K. Peterson, "Angular distributions of secondary electrons caused by electron impact on helium," in Electronic and Atomic Collisions (North-Holland, Amsterdam, 1971), pp. 872-4.

J. P. Cassinelli and D. G. Hummer, "Radiative transfer in spherically symmetric systems -- II. The non-conservative case and linearly polarized radiation," Monthly Notices Roy. Astron. Soc. (in press).

R. J. Celotta, R. A. Bennett and J. L. Hall, "Molecular photodetachment spectrometry," in Electronic and Atomic Collisions (North-Holland, Amsterdam, 1971), pp. 179-81.

J. Cooper, (S. Klarsfeld and G. K. Oertel), "Classical path broadening functions for a Debye-shielded interaction," JILA Report No. 107 (March 17, 1971).

J. Cooper, (E. W. Smith) and W. R. Chappell, "An adiabatic treatment of ion dynamics for forbidden line profiles," Phys. Letters 34A, 363 (1971).

E. A. Enemark and A. Gallagher, "Electron excitation cross section and polarization of sodium resonance radiation," in Electronic and Atomic Collisions (North-Holland, Amsterdam, 1971), pp. 693-5.

J. M. Evans and J. Cooper, "Determination of van der Waals broadening at temperatures of astrophysical interest," J. Quant. Spectrosc. Radiat. Transfer (in press).

S. Geltman, "A high energy approximation I. Proton-hydrogen charge transfer," J. Phys. B (in press).

S. Geltman and M. B. Hidalgo, "A high energy approximation II. Hydrogen atom excitation by electrons," J. Phys. B (in press).

M. B. Hidalgo and S. Geltman, "Theory of fine structure transitions in excited rubidium atoms colliding with rare gas atoms," J. Phys. B (submitted).

J. S. Hildum, "Fabry-Perot deconvolution in the presence of an unknown continuum," Appl. Opt. (in press).

J. S. Hildum and J. Cooper, "Stark broadening of calcium ion resonance lines," Phys. Letters 36A, 153 (1971).

L. J. Kieffer, "Low-energy electron-collision cross section data. Part III. Total scattering, differential elastic scattering," Atomic Data 2, 293 (1971).

L. J. Kieffer, G. M. Lawrence and J. H. Slater, "The dissociative ionization of O_2," in Electronic and Atomic Collisions (North-Holland, Amsterdam, 1971), pp. 574-5.

D. Norcross, "Low energy elastic scattering of electrons by Li and Na," J. Phys. B (in press).

C. B. Opal, E. C. Beaty, and W. K. Peterson, "Tables of energy and angular distributions of electrons ejected from simple gases by electron impact," JILA Report No. 108 (May 26, 1971).

G. Sinnott and E. C. Beaty, "O_3^- photodetachment study using a tunable dye laser," in Electronic and Atomic Collisions (North-Holland, Amsterdam, 1971), pp. 176-8.

P. O. Taylor and G. H. Dunn, "Crossed beam measurement of the cross sections for electron impact excitation of the H and K lines of Ca II," in Electronic and Atomic Collisions (North-Holland, Amsterdam, 1971), pp. 696-8.

(P. Freymuth) and M. S. Uberoi, "Structure of temperature fluctuations in the turbulent wake behind a heated cylinder," Phys. Fluids (in press).

(J. P. Narain) and M. S. Uberoi, "Magnetohydrodynamics of a drop," Phys. Fluids (in press).

(J. P. Narain) and M. S. Uberoi, "Magnetohydrodynamics of conical flows," Phys. Fluids (in press).

(J. P. Narain) and M. S. Uberoi, "A line sink in uniform magnetic field," Phys. Fluids (in press).